PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In the present paper, results demonstrating the significant advantages of matrix-assisted laser desorption/ionization (MALDI) anal. of whole cell samples of bacteria grown on double isotopically-depleted (13C and 15N) media are presented. It is shown that several advantages accrue for MALDI with a 9.4 T Fourier transform mass spectrometer (FTMS). Of particular note, for anal. of whole cells, sample preparation is simple and chemical interference is reduced. Moreover, ion coalescence problems are minimized, and data-base identification of proteins facilitated. Furthermore, high resolution mass spectra obtained from such whole cells show significant improvement in apparent mass resolving power and mass measurement accuracy, whether time-of-flight or FTMS MALDI is used. As a consequence, it becomes possible to detect subtle details in the chemical of the organism, such as the presence of both post-translationally modified and unmodified versions of the same proteins. This approach is also adaptable to direct assay of over-expressed proteins from Escherichia coli cultures and should facilitate studies aimed at the detection of medically important cellular biomarker proteins. REFERENCE COUNT: 43

FILE 'CAPLUS' ENTERED AT 12:06:39 ON 31 MAY 2005
L1 0 (FTMS OR ("FOURIER TRANSFORM" (3A) (MASS (2A) SPECTR?)))(S) "PEAK PROFILE"
L2 2 (FTMS OR ("FOURIER TRANSFORM" (3A) (MASS (2A) SPECTR?))) AND "PEAK PROFILE"
L3 328 (FTMS OR ("FOURIER TRANSFORM" (3A) (MASS (2A) SPECTR?))) (S) (BLOOD OR URINE OR COMPLEX OR BIOLOGIC?)
L4 4 L3 AND WHOLE
L5 0 "INTACT CELL MASS SPECTROMETRY" AND ("FOURIER TRANSFORM" OR FT)
L6 6 "INTACT CELL MASS SPECTROMETRY"

L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:590347 CAPLUS
DOCUMENT NUMBER: 129:220858
TITLE: Identification of pollutants in a municipal well using high resolution mass spectrometry
AUTHOR(S): Grange, Andrew H.; Sovocool, G. Wayne; Donnelly, Joseph R.; Genicola, Floyd A.; Gurka, Donald F.
CORPORATE SOURCE: Environmental Sciences Division, USEPA, NERL, Las Vegas, NV, 89193-3478, USA
SOURCE: Rapid Communications in Mass Spectrometry (1998), 12(17), 1161-1169
CODEN: RCMSEF; ISSN: 0951-4198
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An elevated incidence of childhood cancer was observed near a polluted site. Trace amts. of several isomeric compds. were detected by gas chromatog./mass spectrometry (GC/MS) in a concentrated extract of municipal well water. No matching library mass spectra were found and Fourier transform IR and NMR analyses were not feasible due to the low concentration of the compds. Mass peak profiling from selected-ion recording data (MPPSIRD) provided the sensitivity and scan speed necessary to acquire mass peak profiles at mass resolns. of 10,000-20,000 for the mol. ion (M+.) and 10 fragment ions as capillary GC peaks eluted. Using a profile generation model (PGM), the elemental composition of the mol. ion was determined from the exact masses and abundances of the M, M + 1, and M + 2 profiles. Fragment ion compns. were determined from their exact masses based on elements in the mol. ion. Exact mass differences between mol. and fragment ions corresponded to unique combinations of atoms for neutral losses. Consequent reduction of the number of possible structures for fragment ions simplified mass spectral interpretation. After inspecting library mass spectra for smaller mols., isomeric structures were hypothesized with cyano and alkylcyano groups attached to tetralin. A literature search found such isomers produced by an industrial polymer synthesis. Three isomers in a standard from polymerization of styrene and acrylonitrile provided the same mass spectra and GC retention times as isomers in the extract.
REFERENCE COUNT: 21

L6 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:4909 CAPLUS
DOCUMENT NUMBER: 137:275166
TITLE: Intact cell mass spectrometry (ICMS) used to type methicillin-resistant Staphylococcus aureus: media effects and inter-laboratory reproducibility
AUTHOR(S): Walker, J.; Fox, A. J.; Edwards-Jones, V.; Gordon, D. B.
CORPORATE SOURCE: Department of Biological Sciences, Manchester Metropolitan University, Manchester, M1 5GD, UK
SOURCE: Journal of Microbiological Methods (2002), 48(2-3), 117-126
CODEN: JMIMDQ; ISSN: 0167-7012
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Intact cell mass spectrometry (ICMS) rapidly analyses the surface composition of microorganisms providing rapid, discriminatory fingerprints for identification and subtyping of important nosocomial pathogens such as methicillin resistant Staphylococcus aureus (MRSA). In this study, ICMS using matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI TOF/MS) was assessed for the identification and subtyping of MRSA. An intra- and inter-laboratory reproducibility study was carried out and the effects of culture media (an important source of variation for ICMS) were also studied. Several media used for the cultural identification of MRSA were examined using a panel of well-characterized staphylococcal isolates (n=26). Six MRSA isolates were analyzed over a 1-mo period for intra-laboratory reproducibility on the same instrument and three different culture media. Spectra were consistent for each isolate between the four expts. on the same culture medium. Individual isolates produced different spectral profiles on different culture

media. Spectra from organisms grown on Columbia blood agar contained more peaks (approx. 120) compared to Columbia agar (approx. 50) and methicillin mannitol salt agar (approx. 25). All 26 staphylococcal isolates were subjected to an inter-laboratory study on two MALDI instruments. For each isolate, the overall spectral profile was the same for each of the two instruments but the baseline threshold values was adjusted due to instrument differences in detector sensitivities. Differences between certain regions of the spectra reproducibly identified isolates belonging to the two major MRSA strains (EMRSA phage group 15 and 16). These results demonstrate ICMS with appropriate media selection is a rapid and reproducible technique for identification and discrimination of MRSA. REFERENCE COUNT: 24

L6 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:891240 CAPLUS
DOCUMENT NUMBER: 134:175119
TITLE: Exploring the limits of bacterial identification by intact cell-mass spectrometry
AUTHOR(S): Evason, D. J.; Claydon, M. A.; Gordon, D. B.
CORPORATE SOURCE: Quality Management Ltd., Bury, Lancashire, UK
SOURCE: Journal of the American Society for Mass Spectrometry (2001), 12(1), 49-54
CODEN: JAMSEF; ISSN: 1044-0305
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The limits of intact cell-mass spectrometry (ICM-MS) were tested with regard to the min. number of bacterial cells detectable and its power to discriminate mixed-bacterial cultures. The technique is a surface anal. tool, as is supported by evidence showing that mass fingerprints correspond to material desorbed directly from the cell wall. The brief exposure to solvents, which occurs during sample preparation, does not extract internal cellular material. Spectra were collected over the m/z range of 500 to 10,000. The UV absorbing matrixes used were found to be highly specific to bacterial gram type: <SYM97>-cyano-4-hydroxycinnamic acid for gram-neg. bacteria and 5-chloro-2-mercaptobenzothiazole for gram-pos. bacteria. This specificity allows mixed cultures of different gram types to be differentiated by ICM-MS. The min. number of cells that could reliably give spectra of sufficient data was 104 cells (107 cells/mL). REFERENCE COUNT: 30

L6 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:276981 CAPLUS
DOCUMENT NUMBER: 133:28182
TITLE: Effects of ion mode and matrix additives in the identification of bacteria by intact cell mass spectrometry
AUTHOR(S): Evason, David J.; Claydon, Martin A.; Gordon, Derek B.
CORPORATE SOURCE: Bio-analytical Research Centre, Manchester Metropolitan University, Manchester, M1 5GD, UK
SOURCE: Rapid Communications in Mass Spectrometry (2000), 14(8), 669-672
CODEN: RCMSEF; ISSN: 0951-4198
PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English
AB Protocols for the identification of bacterial cells by intact cell matrix-assisted laser desorption/ionisation time-of-flight mass spectrometry (ICM-TOFMS) are presented. A mass range of 500 to 10 000 m/z is used. The use of formic acid and the crown ether 1, 4, 7, 10, 13, 16-hexaoxacyclooctadecane (18-crown-6) is described. Crown ether is useful for removing metal ion adducts, which degrade spectral purity, and formic acid promotes pos. ions, improves spectral signal, and, hence, increases identification certainty. REFERENCE COUNT: 28

L6 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:203555 CAPLUS
DOCUMENT NUMBER: 133:161505
TITLE: Rapid discrimination between methicillin-sensitive and methicillin-resistant Staphylococcus aureus by intact cell mass spectrometry
AUTHOR(S): Edwards-Jones, Valerie; Claydon, M. A.; Evason, D. J.; Walker, J.; Fox, A. J.; Gordon, D. B.
CORPORATE SOURCE: Department of Biological Sciences, Manchester Metropolitan University, Manchester, M1 5GD, UK
SOURCE: Journal of Medical Microbiology (2000), 49(3), 295-300
CODEN: JMMIAV; ISSN: 0022-2615
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Rapid, accurate discrimination between methicillin-sensitive Staphylococcus aureus (MSSA) and methicillin-resistant S. aureus (MRSA) strains was essential for appropriate therapeutic management and timely intervention for infection control. A rapid method involving intact cell mass spectrometry (ICMS) is presented that shows promise for identification, discrimination of MSSA from MRSA and typing. In ICMS, cells from a bacterial colony are emulsified in a chemical matrix, added to a sample slide, dried and analyzed by matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF-MS). This technique examines the chemical of the intact bacterial cell surface, yielding spectra consisting of a series of peaks from 500 to 10 000, which represent the mass:charge (m:z) ratios. Each peak corresponds to a mol. fragment released from the cell surface during laser desorption. Specimens can be prepared in a few seconds from plate cultures and a spectrum can be obtained within 2 min. ICMS spectra for 20 staphylococcal isolates showed characteristic peaks, some of which were conserved at species level, some at strain level and some were characteristic of the methicillin susceptibility status of the strain. ICMS may have potential for MRSA identification and typing, and may improve infection control measures.
REFERENCE COUNT: 17

10657810

FILE 'CAPLUS' ENTERED AT 19:23:52 ON 19 MAY 2005
L1 63 CELL? (S) (FTMS OR FTICRMS)
L2 5 L1 AND PROFIL?
L3 20 L1 AND (POPULAT? OR BIOLOG? OR PROTEIN? OR DNA)
L4 7 ((WHOLE OR SINGLE OR POPULATION?) (3A) CELL?) AND (FTMS OR FTICRMS)
L5 4 BACTER? (S) (FTMS OR (FOURIER (2A) MALDI) OR FTICRMS)
L6 0 (CELL (2A) POPULAT?) (S) (FTMS OR (FOURIER (2A) MALDI) OR FTICRMS)
L7 0 (CELL (2A) POPULAT?) AND (FTMS OR (FOURIER (2A) MALDI) OR FTICRMS)
L8 9 PROFIL? (S)(FTMS OR (FOURIER (2A) MALDI) OR FTICRMS)

L2 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:921563 CAPLUS
DOCUMENT NUMBER: 142:51636
TITLE: Strategies and data analysis techniques for lipid and phospholipid chemistry elucidation by intact cell MALDI-FTMS
AUTHOR(S): Jones, Jeffrey J.; Stump, Michael J.; Fleming, Richard C.; Lay, Jackson O.; Wilkins, Charles L.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR, USA
SOURCE: Journal of the American Society for Mass Spectrometry (2004), 15(11), 1665-1674
CODEN: JAMSEF; ISSN: 1044-0305
PUBLISHER: Elsevier Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Ions attributed to lipids and phospholipids are directly observed by desorption from whole bacteria using intact cell (IC) matrix-assisted laser desorption-ionization (MALDI) Fourier transform mass spectrometry (FTMS). Saccharomyces cerevisiae are grown in rich media broth, concentrated, and applied directly to the MALDI surface without lysis or chemical treatment. FTMS of MALDI ions gives excellent signal to noise ratios with typical resolving powers of 90,000 and mass precision better than 0.002 Da. Use of accurate mass measurements and a simple set of rules allow assignment of major peaks into one of twelve expected lipid classes. Subsequently, fractional mass vs. whole number mass plots are employed to enhance visual interpretation of the high-resolution data and to facilitate detection of related ions such as those representing homologous series or different degrees of unsatn. This approach, coupled with rules based on bacterial biochem., is used to classify ions with m/z up to about 1000. Major spectral peaks in the range m/z 200-1000 are assigned as lipids and phospholipids. In this study, it is assumed that biol.-derived ions with m/z values lower than 1000 are lipids. This is not unreasonable in view of the facts that mol. wts. of lipids are almost always less than 1000 Da, that the copy nos. for lipids in a cell are higher than those for any single protein

or other component, and that lipids are generally collections of distinct homologous partners, unlike proteins or other cell components. This paper presents a new rapid lipid-profiling method based on IC MALDI-FTMS. REFERENCE COUNT: 43

L2 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:251638 CAPLUS
DOCUMENT NUMBER: 141:273755
TITLE: A top-down method for the determination of residue-specific solvent accessibility in proteins
AUTHOR(S): Novak, Petr; Kruppa, Gary H.; Young, Malin M.; Schoeniger, Joe
CORPORATE SOURCE: Sandia National Laboratories, Livermore, CA, 94551-0969, USA
SOURCE: Journal of Mass Spectrometry (2004), 39(3), 322-328
CODEN: JMSPFJ; ISSN: 1076-5174
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We present a method employing top-down Fourier transform mass spectrometry (FTMS) for the rapid profiling of amino acid side-chain reactivity. The reactivity of side-chain groups can be used to infer residue-specific solvent accessibility and can also be used in the same way as H/D exchange reactions to probe protein structure and interactions. We probed the reactivity of the N-terminal and <SYM101>-lysine amino groups of ubiquitin by reaction with N-hydroxysuccinimidyl acetate (NHSAc), which specifically acetylates primary amines. Using a hybrid Q-FTMS instrument, we observed several series of multiply acetylated ubiquitin ions that varied with the NHSAc: protein stoichiometry. We isolated and fragmented each member of the series of acetylated ubiquitin ions in the front end of the instrument and measured the fragment ion masses in the FTMS analyzer cell to determine which residue positions were modified. As we increased the NHSAc: protein stoichiometric ratio, identification of the fragments from native protein and protein with successively increasing modification allowed the assignment of the complete order of reactivity of the primary amino groups in ubiquitin (Met 1 <SYM187> Lys 6 <SYM187> Lys 48 <SYM187> Lys 63 > Lys 33 > Lys 11 > Lys 27, Lys 29). These results are in excellent agreement with the reactivity expected from other studies and predicted from the known crystal structure of ubiquitin. The top-down approach eliminates the need for proteolytic digestion, high-performance liquid chromatog. sepns. and all other chemical steps except the labeling reaction, making it rapid and amenable to automation using small quantities of protein.
REFERENCE COUNT: 28

L2 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:110009 CAPLUS
DOCUMENT NUMBER: 138:267889
TITLE: Investigation of MALDI-TOF and FT-MS techniques for analysis of Escherichia coli whole cells
AUTHOR(S): Jones, Jeffrey J.; Stump, Michael J.; Fleming, Richard C.; Lay, Jackson O., Jr.; Wilkins, Charles L.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR, 72701, USA
SOURCE: Analytical Chemistry (2003), 75(6), 1340-1347
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Recently, it has been demonstrated that bacteria can be characterized using whole cells and matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS). However, identification of specific bacterial proteins usually requires anal. of cellular fractions or purified exts. Here, the first application of Fourier transform mass spectrometry (FTMS) to anal. of bacterial proteins directly from whole cells is reported. It is shown that accurate mass MALDI-FTMS can be used to characterize specific ribosomal proteins directly from Escherichia coli cells . High-accuracy mass measurements and high-resolution isotope profile data confirm post-translational modifications proposed previously on the basis of low-resolution mass measurements. Seven ribosomal proteins from E. coli whole cells were observed with errors of less than 27 ppm. This was accomplished directly from whole cells without fractionation, concentration, or overt overexpression of characteristic cellular proteins. MALDI-FTMS also provided information regarding E. coli lipids in the low-mass region. Although ions with m/z values below 1000 have been observed by FTMS of whole cells, this represents the first report of detection of ions in the 5000 to 10 000 m/z range by MALDI-FTMS using whole cells. REFERENCE COUNT: 42

L3 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:389900 CAPLUS
DOCUMENT NUMBER: 137:30149
TITLE: Micro-high-performance liquid chromatography/Fourier transform mass spectrometry with electron-capture dissociation for the analysis of protein enzymatic digests
AUTHOR(S): Davidson, Walter; Frego, Lee
CORPORATE SOURCE: Research and Development Center, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA
SOURCE: Rapid Communications in Mass Spectrometry (2002), 16(10), 993-998
CODEN: RCMSEF; ISSN: 0951-4198
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Electron-capture dissociation (ECD) Fourier transform mass spectrometry (FTMS) employed to generate comprehensive sequence information for the chromatog. anal. of enzymic protein digests is described. A pepsin digest of cytochrome c was separated by reversed-phase micro-high-performance liquid chromatog. (<SYM109>HPLC) and ionized "online" by electrospray ionization (ESI). The ions thus formed were transferred to and trapped in the FTMS analyzer cell. Typically, no precursor ion isolation was performed. The trapped ions were subjected to a pulse of electrons to induce

fragmentation. Mass spectra were acquired continuously to produce a three-dimensional LC/MS data set. The spectra were dominated by c and, to a lesser degree, z ions, which provided near complete sequence coverage. External calibration provided good mass accuracy and resolution, typical of FTMS. Thus <SYM109>HPLC/ECD - FTMS is shown to be a highly informative method for the anal. of enzymic protein digests.
REFERENCE COUNT: 21

L3 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:410719 CAPLUS
DOCUMENT NUMBER: 127:78093
TITLE: Quantification of Biomolecules by External Electrospray Ionization Fourier Transform Mass Spectrometry
AUTHOR(S): Padley, Henry R.; Bashir, Sajid; Wood, Troy D.
CORPORATE SOURCE: Department of Chemistry Natural Sciences and Mathematics Complex, State University of New York at Buffalo, Buffalo, NY, 14260-3000, USA
SOURCE: Analytical Chemistry (1997), 69(15), 2914-2918
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Fourier transform mass spectrometry (FTMS) is well-known for its capabilities in structural characterization of mols. Recent developments in radio frequency excitation, linearized trapping, and accumulation of ions generated from external sources have improved the potential of FTMS for quant. anal. Here, a com. external electrospray ionization FTMS, employing a linearized ion trap (the Infinity Cell) and an ion accumulation procedure in which ions are deflected off-axis and injected into the trap, was evaluated as an anal. method for quantifying amino acids, peptides, and proteins. Linear response over .apprx.2-3 orders of magnitude is observed for singly-charged ions with low coeffs. of variation (generally <10%), and the calibration curves generated can be used to quantify structurally similar analytes with <4% relative error, as shown here for quantification of leucine enkephalin from curves generated by methionine enkephalin. Similar precision was obtained for multiply-charged lysozyme, but over only 1.5 orders of magnitude. Some m/z discrimination was observed as a function of trap accumulation potential for a 2-component cytochrome c/lysozyme mixture The results are promising because they suggest that quantification using liquid chromatog. coupled to electrospray FTMS is possible.

L3 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:158908 CAPLUS
TITLE: Modular Fourier transform mass spectrometer for ultrahigh resolutin ESI and MALDI analysis of biomolecules.
AUTHOR(S): Mclver, Robert T.; Li, Yunzhi; Hunter, Richard L.
CORPORATE SOURCE: IonSpec Corporation, Irvine, CA, USA
SOURCE: Book of Abstracts, 213th ACS National Meeting, San Francisco, April 13-17 (1997), ANYL-215. American Chemical Society: Washington, D. C.

CODEN: 64AOAA
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB Matrix-assisted laser desorption/ioization (MALDI) and Electrospray ionization (ESI) mass spectrometry have become important techniques for determining the mol. wts. and structures of peptides, proteins, glycoproteins, and oligonucleotides. Most manufacturers of MALDI mass spectrometers use time-of-flight analyzers, and most manufacturers of ESI instruments use quadrupole mass analyzers. During the last two years, however, IonSpec Corporation has concentrated on developing an alternative approach with Fourier transform detection that is useful for both MALDI and ESI. The IonSpec approach is also unique in that it utilizes an external ion source and a patented RF quadrupole ion guide for transporting ions efficiently from the source to the FTMS analyzer cell. Recent exptl. results from our laboratory have demonstrated four important capabilities of this technique for MALDI and ESI.

L3 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:321277 CAPLUS
DOCUMENT NUMBER: 125:4786
TITLE: High-Resolution MALDI Fourier Transform Mass Spectrometry of Oligonucleotides
AUTHOR(S): Li, Yunzhi; Tang, Kai; Little, Daniel P.; Koester, Hubert; Hunter, Richard L.; McIver, Robert T., Jr.
CORPORATE SOURCE: IonSpec Corporation, Irvine, CA, 18009-F, USA
SOURCE: Analytical Chemistry (1996), 68(13), 2090-2096
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The matrix-assisted laser desorption/ionization (MALDI) method has been used with an external ion source Fourier transform mass spectrometer (FTMS) to analyze single-stranded, mixed-base oligomers of DNA. It is demonstrated that ultrahigh mass resolution (830,000 fwhm) can be achieved for small oligomers, and high resolution (136,000 fwhm) can be achieved for a 25-mer at m/z 7634. MALDI-FTMS can clearly sep. the mol. ion peaks from analyte-matrix adduct peaks and alkali metal-containing species that result from replacement of hydrogen ions with sodium or potassium ions at multiple sites along the phosphate backbone. Previous MALDI-FTMS studies of oligonucleotides had two limitations: (1) low sensitivity due to difficulty in trapping the high kinetic energy ions made by the laser and (2) fragmentation of the ions due to the long delay (tens to hundreds of milliseconds) between their formation and detection. Both of these problems are alleviated in the present study. With the external ion source FTMS instrument, ions made by MALDI are injected at low energy into the analyzer cell by a rf-only quadrupole ion guide, captured by gating the voltage on the trapping plates, and cooled by a 0.5-s pulse of argon gas. Under these conditions, fragmentation is minimized, and DNA ions can be trapped in the FTMS analyzer cell for greater than 50 s. Sensitivity is also improved, as demonstrated by detection of 1 pmol of a single-stranded, mixed-base 20-mer of DNA, with a signal-to-noise ratio greater than 20:1.

L3 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:338833 CAPLUS
DOCUMENT NUMBER: 122:127859
TITLE: Peptide amino acid sequence analysis using matrix-assisted laser desorption/ionization and fourier transform mass spectrometry
AUTHOR(S): Castoro, John A.; Wilkins, Charles L.; Woods, Amina S.; Cotter, Robert J.
CORPORATE SOURCE: Dept. Chem., Univ. California at Riverside, Riverside, CA, 92521, USA
SOURCE: Journal of Mass Spectrometry (1995), 30(1), 94-8
CODEN: JMSPFJ; ISSN: 1076-5174
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB High-performance matrix-assisted laser desorption/ionization (MALDI) using 7 T Fourier transform mass spectrometry (FTMS) was investigated for peptide amino acid sequence anal. Two synthetic peptides representative of the type which would be displayed by major histocompatibility complex mols. from tumor cells were investigated by MALDI/FTMS . Mol. ions of the two 9-amino acid peptides were detected with resolving power of 8000-17,900 and mass measurement accuracy between 8 and 81 ppm for the all 12C isotope ions. An ultra-high resolution spectrum (RP 300,000) for the mol. ion of one of the two peptides was obtained. Structurally useful sequence information was obtained by use of surface-induced dissociation (SID) of the mol. ion species. Interestingly, SID of a sodium-attached peptide mol. ion resulted in the production of numerous sodium-attached sequence ions.

L3 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:625574 CAPLUS
DOCUMENT NUMBER: 121:225574
TITLE: Detection limits for matrix-assisted laser desorption of polypeptides with an external ion source Fourier-transform mass spectrometer
AUTHOR(S): Li, Yunzhi; McIver, Robert T., Jr.
CORPORATE SOURCE: Dep. Chem., Univ. California, Irvine, CA, 92717, USA
SOURCE: Rapid Communications in Mass Spectrometry (1994), 8(9), 743-9
CODEN: RCMSEF; ISSN: 0951-4198
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Sensitivity in the low-femiomole range with mass resolution greater than 20000 is demonstrated for several polypeptides analyzed by a mass spectrometer that pairs matrix-assisted laser desorption/ionization (MALDI) and Fourier-transform mass spectrometry (FTMS). The compds. investigated were substance P, renin substrate, melittin, the B-chain of the bovine insulin, and bovine insulin. Standard solns. of the polypeptides were prepared with 30% acetonitrile + water, and micropipettes were used to transfer small amts. (1-20 fmol) to a sample probe. The samples were embedded in a large excess of matrix material (2,5-dihydroxybenzoic acid) and ionized by a pulse from an excimer laser. The FTMS instrument used for these expts. has the MALDI source in a sep.

chamber outside the magnetic field. Ions are extracted from the source and transported by an RF-only quadrupole ion guide to an FTMS analyzer cell mounted in the homogeneous region of a 6.5 T supercond. magnet. The high sensitivity of MALDI-FTMS is due, in part, to the high transfer efficiency of the ion guide, even for ions with a wide range of kinetic energies. The ion guide is easy to use because there are only two adjustments (RF amplitude and DC offset voltage), and unlike electrostatic ion transport means, alignment of it with the axis of the magnetic field is not critical The mass resolution and sensitivity of MALDI-FTMS is compared with that of MALDI done with time-of-flight, magnetic sector, and quadrupole ion-trap mass spectrometers.

L3 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:453256 CAPLUS
DOCUMENT NUMBER: 121:53256
TITLE: High-resolution characterization of biomolecules by using an electrospray ionization Fourier-transform mass spectrometer
AUTHOR(S): Winger, Brian E.; Hein, Richard E.; Becker, Bruce L.; Campana, Joseph E.
CORPORATE SOURCE: Extrel FTMS, Waters, Madison, WI, 53711-2424, USA
SOURCE: Rapid Communications in Mass Spectrometry (1994), 8(6), 49507
CODEN: RCMSEF; ISSN: 0951-4198
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors report a new electrospray ionization (ESI) Fourier-transform mass spectrometer (FTMS) based on their 3 T Model 2001 FTMS system that uses their new external source accessory, UltraSource, to transport ions generated in the ESI source into the trapped-ion cell. The UltraSource is attached on the side of the superconducting magnet that is opposite the laser probe accessories, allowing for ESI and laser desorption techniques to be done on the same system without need for changeover. Bovine ubiquitin was studied as an example.

L3 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:404308 CAPLUS
DOCUMENT NUMBER: 121:4308
TITLE: High-Accuracy Molecular Mass Determination for Peptides and Proteins by Fourier Transform Mass Spectrometry
AUTHOR(S): Li, Yunzhi; McIver, Robert T., Jr.; Hunter, Richard L.
CORPORATE SOURCE: Department of Chemistry, University of California, Irvine, CA, 92717, USA
SOURCE: Analytical Chemistry (1994), 66(13), 2077-83
CODEN: ANCHAM; ISSN: 0003-2700
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new calibration method has been developed for Fourier transform mass spectrometry (FTMS) that is accurate to better than 0.001% (10 ppm) for peptides and proteins up to 5700 Da. The custom-designed FTMS instruments used for this work have

a matrix-assisted laser desorption/ionization (MALDI) source located outside of the magnetic field in a differentially pumped chamber, and ions are injected through the fringing fields of the magnet into the FTMS analyzer cell by a long quadrupole ion guide. The mass spectrometer is calibrated with four model compds. ([Arg8]-vasopressin, melittin, bovine insulin B-chain, and bovine insulin) of known mol. mass. The set of measured ion resonance frequencies (f) for these compds. are fit to a three-term calibration equation of the form $f = A(z/m) + B(V) + C(V2)(m/z)$, where m/z is the mass-to-charge ratio of a calibrant peak, V is the trapping voltage, and A, B, and C are calibration coeffs. that depend on the magnetic field strength and the dimensions of the analyzer cell. The same set of calibration coeffs. can be used for many weeks because the magnet and the electronics of the FTMS instrument are very stable. This method is useful because unknowns can be run sep. without the need to add an internal calibration compound in with the sample.

L3 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:318599 CAPLUS
DOCUMENT NUMBER: 120:318599
TITLE: FTMS method for high resolution matrix-assisted laser desorption
AUTHOR(S): McIver, Robert T., Jr.; Li, Yunzhi; Hunter, Richard L.
CORPORATE SOURCE: Dep. Chem., Univ. California, Irvine, CA, 92717, USA
SOURCE: International Journal of Mass Spectrometry and Ion Processes (1994), 132(3), L1-L7
CODEN: IJMPDN; ISSN: 0168-1176
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A Fourier transform mass spectrometer with an external ion source has been modified for use with matrix-assisted laser desorption. High trapping potentials on the FTMS analyzer cell decelerate and trap the laser-produced ions, and a pulsed argon buffer gas cools them prior to detection. For gramicidin S, only one laser pulse is needed to produce mass spectra with a high signal-to-noise ratio and a mass resolution of 1100000 (FWHM). Several other oligopeptides and small proteins have been analyzed, including bovine insulin that was detected at a mass resolution of 90000. These results represent the highest mass resolution ever demonstrated for ions made by MALDI.

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
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TITLE: Use of double-depleted 13C and 15N culture media for analysis of whole cell bacteria by MALDI time-of-flight and Fourier transform mass spectrometry
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